Atomic CP-violating polarizability

Boris Ravaine,[1] M. G. Kozlov,[2,*] and Andrei Derevianko[1,†]

[1] *Department of Physics, University of Nevada, Reno, Nevada 89557*
[2] *Petersburg Nuclear Physics Institute, Gatchina 188300, Russia*

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Searches for CP violating effects in atoms and molecules provide important constrains on competing extensions to the standard model of elementary particles. In particular, CP violation in an atom leads to the CP-odd (T,P-odd) polarizability $\beta^{\rm CP}$: a magnetic moment $\mu^{\rm CP}$ is induced by an electric field $\mathcal{E}_0$ applied to an atom, $\mu^{\rm CP} = \beta^{\rm CP}\mathcal{E}_0$. We estimate the CP-violating polarizability for rare-gas (diamagnetic) atoms He through Rn. We relate $\beta^{\rm CP}$ to the permanent electric dipole moment (EDM) of the electron and to the scalar constant of the CP-odd electron-nucleus interaction. The analysis is carried out using the third-order perturbation theory and the Dirac-Hartree-Fock formalism. We find that, as a function of nuclear charge Z, $\beta^{\rm CP}$ scales steeply as $Z^5R(Z)$, where slowly-varying $R(Z)$ is a relativistic enhancement factor. Finally, we evaluate a feasibility of setting a limit on electron EDM by measuring CP-violating magnetization of liquid Xe. We find that such an experiment could provide competitive bounds on electron EDM only if the present level of experimental sensitivity to ultra-weak magnetic fields [Kominis *et al.*, Nature **422**, 596 (2003)] is improved by several orders of magnitude.

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I. INTRODUCTION

The existence of a permanent electric dipole moment (EDM) of a particle simultaneously violates two discrete symmetries: parity (P) and time reversal (T). By the virtue of the CPT-theorem, the T-violation would imply CP-violation [1, 2]. While no EDMs have been found so far, most supersymmetric extensions of the Standard Model of elementary particles predict electron EDMs, d_e, that are within a reach of planned and on-going experimental searches. Here we investigate a related T-odd, P-odd quantity — CP-violating polarizability, $\beta^{\rm CP}$, introduced recently by Baryshevsky [3]. For a diamagnetic atom, a non-vanishing $\beta^{\rm CP}$ could provide an unambiguous signature of the electron EDM or other CP-violating mechanisms. Here we relate $\beta^{\rm CP}$ to d_e via *ab initio* relativistic calculations for closed-shell atoms. We also relate $\beta^{\rm CP}$ to the scalar constant of the CP-odd electron-nucleus interaction.

An interaction of an atom with external DC electric field in the presence of the electron EDM causes spin polarization in the direction of the field [4]. The first attempt to measure corresponding magnetization of the ferromagnetic crystal was made by Vasiliev and Kolycheva in 1978 [5]. According to Lamoreaux [6], modern techniques allow to improve that old measurement by many orders of magnitude and reach the sensitivity, which allows to improve present limit on the electron EDM [7]:

$$d_e\,(\mathrm{Tl}) < 1.6 \times 10^{-27} e \cdot \mathrm{cm}.$$

First results of the new generation of experiments with ferromagnetic solids were recently reported by Hunter [8]. Characteristic feature of the experiments with macroscopic magnetization is the dependence of the signal on the density of atoms. That gives a huge enhancement in sensitivity for a condensed phase sample.

It is generally assumed that diamagnetic atoms are not useful for the search of the electron EDM. However, Baryshevsky has recently pointed out [3] that CP-violating magnetization would also exists for a diamagnetic atom. For a spherically-symmetric atom, the E-field-induced magnetic moment $\mu^{\rm CP}$ can be expressed in terms of CP-violating polarizability $\beta^{\rm CP}$ as

$$\mu^{\rm CP} = \beta^{\rm CP}\mathcal{E}_0, \tag{1}$$

where $\mathcal{E}_0$ is the strength of the electric field. This observation opens new experimental possibilities. For example, one can measure magnetization of liquid xenon in a strong external electric field. The advantage of the experiment with diamagnetic liquid in comparison to ferromagnetic solids is a much lower magnetic noise.

For a diamagnetic (closed-shell) atom the magnetization (1) appears in the higher orders of the perturbation theory than for the open-shell atoms. In this paper we calculate polarizability $\beta^{\rm CP}$ for rare-gas atoms He through Rn using third-order perturbation theory and Dirac-Hartree-Fock (DHF) formalism.

Further, we evaluate a feasibility of setting a limit on electron EDM by measuring CP-violating magnetization of liquid Xe (LXe). We consider the effect of the environment on $\beta^{\rm CP}$ of Xe atoms in LXe. We use a simple cell model of an atom confined in a spherically-symmetric cavity [9]. In a non-polar liquid, such a cavity roughly approximates an averaged interaction with the neighboring atoms. We solve the DHF equations with proper boundary conditions at the cavity radius. For LXe, we find that compared to the CP-odd polarizability of an

*Electronic address: mgk@MF1309.spb.edu
†Electronic address: andrei@unr.edu

isolated atom, the resulting CP-odd polarizability of an atom of LXe is suppressed by about 65%.

We find that the CP-violating polarizability exhibits an unusually strong dependence on the nuclear charge Z. Previously, Sandars [10, 11] has shown that an atomic enhancement factor for the electron EDM is of the order of $\alpha^2 Z^3$, where $\alpha \approx 1/137$ is the fine structure constant. As we demonstrate below, for a diamagnetic atom, the polarizability $\beta^{\rm CP}$ vanishes in the non-relativistic approximation. Because of that it is suppressed by a factor of $(\alpha Z)^2$. With the Sandars' enhancement factor this leads to a steep, Z^5, scaling of the effect.

Recently there was a renewed interest to the CP-odd weak neutral current interactions of electrons with nucleons [12]. It is known that in atomic experiments the electron EDM is indistinguishable from the scalar CP-odd weak neutral currents [1, 13]. Any new limit on the electron EDM from the atomic experiments will also lead to the improved limit on the scalar constant of the CP-odd electron-nuclear interaction. Here we relate computed $\beta^{\rm CP}$ to the scalar constant of the CP-odd electron-nucleus interaction.

The paper is organized as follows: In Section II we derive the third-order expression for the CP-violating polarizability and use the independent-particle approximation to simplify the atomic many-body expressions. In Section III we present results of our DHF calculations of $\beta^{\rm CP}$ for rare-gas atoms and derive the Z-scaling of $\beta^{\rm CP}$. In Section IV we evaluate a feasibility of setting a limit on electron EDM by measuring CP-violating magnetization of liquid Xe. Finally, in Section V we draw conclusions. Unless specified otherwise, atomic units $|e| = \hbar = m_e \equiv 1$ and Gaussian system for electromagnetic equations are used throughout. In these units, the Bohr magneton is $\mu_B = \alpha/2$ and the unit of magnetic field is $m_e^2 e^5/\hbar^4 \approx 1.72 \times 10^7$ Gauss.

II. FORMALISM

In this Section we derive the expression for CP-violating polarizability within the third-order perturbation theory. Further, we simplify the derived expression using the Dirac-Hartree-Fock approximation for atomic many-body states.

The problem to be solved can be formulated as follows: What is the induced magnetic moment $\langle \boldsymbol{\mu} \rangle$ of an atom perturbed by an external electric field $\mathcal{E}_0$? It is easy to demonstrate that if the atomic wavefunctions are the eigenstates of the parity and time-reversal operators, the induced magnetic moment vanishes. However, in the presence of the CP-odd interactions, $V^{\rm CP}$, there appears a tiny E-field-induced magnetic moment. To emphasize the essential role of CP-violation in the generation of the magnetic-moment, we will use CP superscript with the magnetic moment, $\langle \boldsymbol{\mu}^{\rm CP} \rangle$. The interaction $V^{\rm CP}$ can be due to electron EDM or CP-odd weak neutral currents, and we will specify the particular forms of $V^{\rm CP}$ in Section II C. For a spherically-symmetric system, the induced magnetic moment will be directed along the applied E-field.

A. Third-order formula for the induced magnetic moment

We develop the perturbative expansion for the atomic wavefunction $|\Psi_0\rangle$ in terms of the combined interaction $W = V^{\rm CP} + V^{\rm ext}$. Here $V^{\rm ext}$ is the interaction with the external electric field applied along the z-axis, $V^{\rm ext} = -D_z \mathcal{E}_0$, D_z being the z-component of the electric dipole moment operator. To estimate the dominant contribution to $\langle \boldsymbol{\mu} \rangle$, it is sufficient to truncate the perturbative expansion for the atomic wavefunction at the second order in W, $|\Psi_0\rangle \approx |\Psi_0^{(0)}\rangle + |\Psi_0^{(1)}\rangle + |\Psi_0^{(2)}\rangle$. Then the expectation value of the magnetic moment reads

$$\langle \boldsymbol{\mu}^{\rm CP} \rangle = \langle \Psi_0^{(1)} | \boldsymbol{\mu} | \Psi_0^{(1)} \rangle + \langle \Psi_0^{(0)} | \boldsymbol{\mu} | \Psi_0^{(2)} \rangle + \langle \Psi_0^{(2)} | \boldsymbol{\mu} | \Psi_0^{(0)} \rangle \,. \tag{2}$$

To arrive at the above expression we used a simplifying fact that the magnetic moment is a P-even operator, while both $|\Psi_0^{(0)}\rangle$ and $|\Psi_0^{(2)}\rangle$ have parities opposite to the one of the first-order correction $|\Psi_0^{(1)}\rangle$.

The textbook expressions for the first and second-order corrections to wavefunctions can be found, for example, in Ref. [14]. With these expressions,

$$\langle \boldsymbol{\mu}^{\rm CP} \rangle = \langle \boldsymbol{\mu}^{\rm CP} \rangle_1 + \langle \boldsymbol{\mu}^{\rm CP} \rangle_2 + \langle \boldsymbol{\mu}^{\rm CP} \rangle_3 \,, \tag{3}$$

$$\langle \boldsymbol{\mu}^{\rm CP} \rangle_1 = 2 \sum_{kl} \frac{V^{\rm CP}_{0k}}{E_0 - E_k} \boldsymbol{\mu}_{kl} \frac{V^{\rm ext}_{l0}}{E_0 - E_l} \,, \tag{4}$$

$$\langle \boldsymbol{\mu}^{\rm CP} \rangle_2 = 2 \sum_{kl} \boldsymbol{\mu}_{0k} \frac{V^{\rm CP}_{kl}\, V^{\rm ext}_{l0}}{(E_0 - E_k)\,(E_0 - E_l)} \,, \tag{5}$$

$$\langle \boldsymbol{\mu}^{\rm CP} \rangle_3 = 2 \sum_{kl} \boldsymbol{\mu}_{0k} \frac{V^{\rm ext}_{kl}\, V^{\rm CP}_{l0}}{(E_0 - E_k)\,(E_0 - E_l)} \,. \tag{6}$$

In these formulas, the summations are carried out over the eigenstates of the atomic Hamiltonian H_a, $H_a|\Psi_p^{(0)}\rangle = E_p|\Psi_p^{(0)}\rangle$. The derived third-order expression can be presented in a more compact and symmetrical form using the resolvent operator $\mathcal{R} = (E_0 - H_a)^{-1}$,

$$\begin{aligned} \langle \boldsymbol{\mu}^{\rm CP} \rangle = {} & 2\langle 0 | V^{\rm CP}\, \mathcal{R}\, \boldsymbol{\mu}\, \mathcal{R}\, V^{\rm ext} | 0 \rangle + \\ & 2\langle 0 | \boldsymbol{\mu}\, \mathcal{R}\, V^{\rm CP} \mathcal{R}\, V^{\rm ext} | 0 \rangle + 2\langle 0 | \boldsymbol{\mu}\, \mathcal{R}\, V^{\rm ext}\, \mathcal{R}\, V^{\rm CP} | 0 \rangle \,. \end{aligned} \tag{7}$$

The three above contributions differ by permutations of the operators $\boldsymbol{\mu}$, $V^{\rm CP}$ and $V^{\rm ext}$.

B. Dirac-Hartree-Fock approximation

Having derived a general third-order expression for the induced magnetic moment, Eq. (7), here we proceed with

the atomic-structure part of the evaluation. We employ the conventional Hartree-Fock (HF) or independent-particle approximation for that purpose. In this approach, the atomic many-body wavefunction is represented by the Slater determinant composed of single-particle orbitals. These orbitals are determined from a set of the HF equations. Using a complete set of Slater determinants, the contributions to the induced magnetic moment, Eq.(4–6), may be expressed as

$$\left\langle \boldsymbol{\mu}^{\rm CP}\right\rangle_{1,a} = 2\sum_{amn}\frac{V^{\rm CP}_{an}\,\boldsymbol{\mu}_{nm}\,V^{\rm ext}_{ma}}{(\varepsilon_m-\varepsilon_a)\,(\varepsilon_n-\varepsilon_a)}\,, \tag{8}$$

$$\left\langle \boldsymbol{\mu}^{\rm CP}\right\rangle_{1,b} = -2\sum_{abm}\frac{V^{\rm CP}_{bm}\,\boldsymbol{\mu}_{ab}\,V^{\rm ext}_{ma}}{(\varepsilon_m-\varepsilon_a)\,(\varepsilon_m-\varepsilon_b)}, \tag{9}$$

$$\left\langle \boldsymbol{\mu}^{\rm CP}\right\rangle_{2,a} = 2\sum_{amn}\frac{\boldsymbol{\mu}_{an}V^{\rm CP}_{nm}\,V^{\rm ext}_{ma}}{(\varepsilon_m-\varepsilon_a)\,(\varepsilon_n-\varepsilon_a)}\,, \tag{10}$$

$$\left\langle \boldsymbol{\mu}^{\rm CP}\right\rangle_{2,b} = -2\sum_{abm}\frac{\boldsymbol{\mu}_{bm}V^{\rm CP}_{ab}\,V^{\rm ext}_{ma}}{(\varepsilon_m-\varepsilon_a)\,(\varepsilon_m-\varepsilon_b)}, \tag{11}$$

$$\left\langle \boldsymbol{\mu}^{\rm CP}\right\rangle_{3,a} = 2\sum_{amn}\frac{\boldsymbol{\mu}_{an}V^{\rm ext}_{nm}\,V^{\rm CP}_{ma}}{(\varepsilon_m-\varepsilon_a)\,(\varepsilon_n-\varepsilon_a)}\,, \tag{12}$$

$$\left\langle \boldsymbol{\mu}^{\rm CP}\right\rangle_{3,b} = -2\sum_{abm}\frac{\boldsymbol{\mu}_{bm}V^{\rm ext}_{ab}\,V^{\rm CP}_{ma}}{(\varepsilon_m-\varepsilon_a)\,(\varepsilon_m-\varepsilon_b)}\,. \tag{13}$$

Here indexes a and b run over single-particle orbitals occupied in $|\Psi_0\rangle$, indexes m and n run over virtual orbitals, and ε_i are the energies of the HF orbitals.

It is well known that the relativistic effects are essential for the non-vanishing contributions to energy levels due to EDMs (Schiff theorem). Moreover, in Section III A, we will demonstrate that the relativism enters into the calculations of CP-violating polarizability in the enhanced fashion: one also needs to incorporate relativistic corrections to electric- and magnetic-dipole matrix elements and energies entering Eq.(4–6). We include the relativistic effects by directly solving Dirac-Hartree-Fock (DHF) equations

$$\left(c(\boldsymbol{\alpha}\cdot\boldsymbol{p})+\beta c^2+V_{\rm nuc}+V_{\rm DHF}\right)u_i(\boldsymbol{r}) = \varepsilon_i u_i(\boldsymbol{r})\,, \tag{14}$$

where $V_{\rm nuc}$ is a potential of the Coulomb interaction with a finite-size nucleus and $V_{\rm DHF}$ is non-local self-consistent DHF potential.

C. Matrix elements

We use the following ansatz for the Dirac bi-spinor

$$u_{n\kappa m}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} iP_{n\kappa}(r)\;\Omega_{\kappa m}(\hat r)\\ Q_{n\kappa}(r)\;\Omega_{-\kappa m}(\hat r)\end{pmatrix}, \tag{15}$$

where P and Q are the large and small radial components respectively and Ω is the spherical spinor. The angular quantum number $\kappa = (l-j)\,(2j+1)$.

In particular, the reduced matrix elements of the magnetic-dipole and electric-dipole moment operators between two bi-spinors are given by

$$\begin{aligned}\langle a||\mu||b\rangle &= \frac{1}{2}\,(\kappa_a+\kappa_b)\;\langle -\kappa_a||C_1||\kappa_b\rangle\times \\ &\int_0^\infty r\;dr\{P_a\,(r)\,Q_b\,(r)+Q_a\,(r)\,P_b\,(r)\}\,,\end{aligned} \tag{16}$$

$$\begin{aligned}\langle a||D||b\rangle &= -\langle\kappa_a||C_1||\kappa_b\rangle\times \\ &\int_0^\infty r\;dr\{P_a\,(r)\,P_b\,(r)+Q_a\,(r)\,Q_b\,(r)\}\,,\end{aligned} \tag{17}$$

$C_1(\hat r)$ being normalized spherical harmonic.

At this point we would like to specify particular forms for the CP-odd interaction $V^{\rm CP}$. We will distinguish between the electron EDM coupling $V^{\rm CP,EDM}$ and weak neutral-current (NC) interactions $V^{\rm CP,NC}$. The EDM interaction of an electron with an electric field $\mathcal{E}_{\rm int}$ can be written in four-component Dirac notation as [13]:

$$V^{\rm CP,EDM} = 2d_e\begin{pmatrix}0 & 0\\ 0 & \boldsymbol{\sigma}\cdot\mathcal{E}_{\rm int}\end{pmatrix}. \tag{18}$$

The matrix element of this interaction is given by

$$V^{\rm CP,EDM}_{ab} = d_e\left\{2Z\int_0^\infty\frac{dr}{r^2}Q_a\,(r)\,Q_b\,(r)\right\}\delta_{\kappa_a,-\kappa_b}\delta_{m_a,m_b}\,, \tag{19}$$

where we assumed that the dominant contribution is accumulated close to the nucleus (of charge Z) so that $\mathcal{E}_{\rm int}$ can be approximated by the nuclear field. The selection rules with respect to angular quantum numbers m and κ arise because $V^{\rm CP}$ is a pseudoscalar.

Recently there was a renewed interest to CP-odd weak neutral current interactions of electrons with nucleons [12]. It is known that in atomic experiments EDM of the electron is indistinguishable from the scalar CP-odd weak neutral currents [13]:

$$\begin{aligned}V^{\rm CP,NC} &= {\rm i}\frac{G_{\rm F}}{\sqrt{2}}(Zk_1^p+Nk_1^n)\gamma_0\gamma_5\rho(\boldsymbol{r}),\\ &\equiv {\rm i}\frac{G_{\rm F}Z}{\sqrt{2}}k_1^{\rm nuc}\gamma_0\gamma_5\rho(\boldsymbol{r}),\end{aligned} \tag{20}$$

where $G_{\rm F}=2.2225\times10^{-14}$ a.u. is the Fermi constant, $k_1^{p,n}$ are dimensionless constants of the scalar P,T-odd weak neutral currents for proton and neutron ($k_1^{\rm nuc}\equiv k_1^p+\frac{N}{Z}k_1^n$). Further, Z and N are the numbers of protons and neutrons in the nucleus, $\gamma_{0,5}$ are Dirac matrices, and $\rho(\boldsymbol{r})$ is the nuclear density.

III. RESULTS FOR RARE-GAS ATOMS

The derived HF expressions hold for any atomic or molecular system with a state composed from a single Slater determinant. Below we will carry out calculations for the rare-gas atoms He through Rn. These closed-shell

atoms have a $^1S_0$ ground state and, due to the spherical symmetry, the CP-violating polarizability is a scalar quantity, i.e., the induced magnetic moment is parallel to the applied electric field. The intermediate many-body states in Eq. (4–6) are particle-hole excitations, with the total angular momenta of $J = 0$ or $J = 1$, depending on the multipolarity of the involved operator.

To carry out the numerical evaluation, we solved the DHF equations in the cavity using a B-spline basis set technique by Johnson et al. [15]. The resulting set of basis functions is finite and can be considered as numerically complete. In a typical calculation we used a set of basis functions expanded over 100 B-splines. An additional peculiarity related to the Dirac equation is an appearance of negative energy states ($\varepsilon_m < -m_e c^2$) in the summation over intermediate states in Eq. (8)–(13). In our calculations we used the so-called length-form of the electric-dipole operator, Eq. (17) and we found the contribution of negative-energy-state to be insignificant.

Atom	Z	$\beta^{\rm CP}/d_e$	$\beta^{\rm CP}/k_1^{\rm nuc}$
He	2	3.8[−9]	2.4[−22]
Ne	10	2.2[−6]	1.5[−19]
Ar	18	7.4[−5]	5.2[−18]
Kr	36	3.6[−3]	3.1[−16]
Xe	54	4.5[−2]	5.3[−15]
Rn	86	1.07	2.2[−13]

TABLE I: CP-violating polarizability, $\beta^{\rm CP}$, in Gaussian atomic units, for rare-gas atoms. CP-violation is either due to the electron EDM, d_e, or due to the neutral currents (20). Notation $x[y]$ stands for $x \times 10^y$.

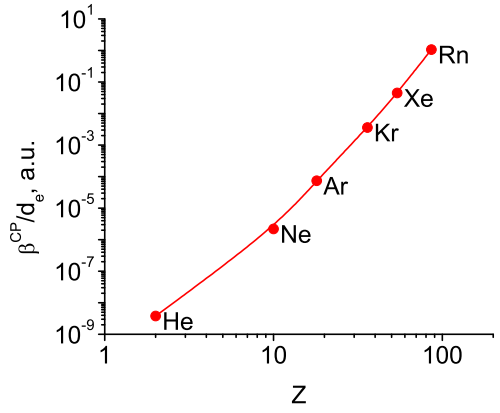

FIG. 1: (Color online) Dependence of the CP-violating polarizability $\beta^{\rm CP}$ on the nuclear charge Z for rare-gas atoms. CP-violation is due to the electron EDM, d_e. The ratio $\beta^{\rm CP}/d_e$ is given in atomic units.

Numerical results for rare-gas atoms are presented in Table I and also plotted in Fig. 1. In Table I, the values in the column marked $\beta^{\rm CP}/d_e$ were computed directly, while the values $\beta^{\rm CP}/k_1^{\rm nuc}$ (the last column) were obtained from $\beta^{\rm CP}/d_e$ as explained in Section III A.

From Fig. 1 we observe a pronounced dependence of the values on the nuclear charge Z. Such a steep scaling of the CP-odd polarizabilities is expected from the considerations presented in Sec. III A.

To illustrate the (doubly) relativistic origin of the CP-odd polarizability $\beta^{\rm CP}$, we compile values of various contributions to $\beta^{\rm CP}$ in Table II for an isolated Xe atom. Apparently, the dominant contributions are from $\langle\mu^{\rm CP}\rangle_{1,a}$, Eq. (8), and $\langle\mu^{\rm CP}\rangle_{1,b}$, Eq. (9), but there is strong cancelation between these two terms. As we will see below, this cancelation is not accidental.

k	$\beta^{\rm CP}_{k,a}/d_e$	$\beta^{\rm CP}_{k,b}/d_e$	sum
1	−0.108	0.132	2.44[−2]
2	6.53[−3]	−6.63[−5]	6.46[−3]
3	8.19[−3]	5.13[−3]	1.33[−2]
total			4.42[−2]

TABLE II: Contributions to CP-violating polarizability, $\beta^{\rm CP}/d_e$, in Gaussian atomic units, for an isolated Xe atom. Each contribution is defined via Eq. (8)–(13) as $\beta^{\rm CP}_{k,\alpha}/d_e = \langle\mu^{\rm CP}\rangle_{k,\alpha}/(d_e\mathcal{E}_0)$. CP-violation is due to the electron EDM, d_e. Notation $x[y]$ stands for $x \times 10^y$.

A. Z^5 scaling and relation between EDM and NC contributions

Let us consider non-relativistic limit of Eqs. (4 – 6). The magnetic moment operator is reduced to the form:

$$\boldsymbol{\mu} = \frac{\alpha}{2}(2\boldsymbol{s} + \boldsymbol{l}). \tag{21}$$

This operator can not change electronic principal quantum numbers. Because of that the contributions (5) and (6) vanish, as there $\boldsymbol{\mu}$ should mix occupied and excited orbitals. Thus, we are left with the single term (4), which can be further split in two parts (8) and (9). We will show now that these two parts cancel each other.

Indeed, in the non-relativistic approximation the operator $V^{\rm CP}$ is given by a scalar product of the spin vector and the orbital vector. Therefore, in the LS-coupling scheme it can couple the ground state $^1S_0$ only with excited states $^3P_0$. Operator (21) is diagonal in the quantum numbers L and S and can couple $^3P_0$ only with $^3P_1$. To return back to the ground state, the dipole operator $V^{\rm ext}$ has to couple $^3P_1$ with $^1S_0$. However, this matrix element vanishes in the non-relativistic approximation. The above states $^3P_{0,1}$ are formed from the excited electron and a whole in the core, which correspond to two expressions (8) and (9). We conclude that these two contributions exactly cancel in the non-relativistic approximation.

The matrix element $\langle {}^3P_1|V^{\rm ext}|{}^1S_0\rangle$ is proportional to the spin-orbit mixing, which is of the order of $(\alpha Z)^2$. It follows from (16) that relativistic correction to operator (21) is of the same order. This correction accounts for the nondiagonal in the principle quantum numbers matrix elements of $\boldsymbol{\mu}$ and leads to the nonzero values of the terms (5) and (6). Thus, we see that all three terms in (3) are suppressed by the relativistic factor $(\alpha Z)^2$, in agreement with numerical results from Table II.

Matrix elements of the CP-odd interaction $V^{\rm CP}$ depend on the short distances and rapidly decrease with quantum number j. To a good approximation it is possible to neglect all matrix elements for $j \geq 3/2$. For the remaining matrix elements between orbitals $s_{1/2}$ and $p_{1/2}$ an analytical expression can be found in [13]:

$$\langle s_{1/2}|V^{\rm CP,EDM}|p_{1/2}\rangle = \frac{16}{3}\frac{\alpha^2 Z^3 R^{\rm EDM}}{(\nu_s\nu_p)^{3/2}}d_e, \qquad (22)$$

$$\langle s_{1/2}|V^{\rm CP,NC}|p_{1/2}\rangle = \frac{G_{\rm F}}{2\sqrt{2}\pi}\frac{\alpha Z^3 R^{\rm NC}}{(\nu_s\nu_p)^{3/2}}k_1^{\rm nuc}, \qquad (23)$$

where we use effective quantum numbers $\nu = (-2\varepsilon)^{-1/2}$. $R^{\rm EDM}$ and $R^{\rm NC}$ are relativistic enhancement factors:

$$R^{\rm EDM} = \frac{3}{\gamma(4\gamma^2-1)} = \begin{cases} 1, & Z=1, \\ 1.4, & Z=54, \ \text{(Xe)}, \\ 2.7, & Z=86, \ \text{(Rn)}, \end{cases} \qquad (24)$$

$$R^{\rm NC} = \frac{4\gamma(2Zr_{\rm N})^{2\gamma-2}}{\Gamma^2(2\gamma+1)} = \begin{cases} 1, & Z=1, \\ 2.5, & Z=54, \\ 8.7, & Z=86, \end{cases} \qquad (25)$$

where $\gamma = \sqrt{1-(\alpha Z)^2}$ and the radius of the nucleus is taken to be $r_{\rm N} = 1.2\,(Z+N)^{1/3}$fm [13].

We see that both CP-odd operators scale as Z^3R with relativistic enhancement factors R given by (24) and (25). This scaling adds up with relativistic suppression $(\alpha Z)^2$ discussed above to give overall scaling Z^5R. This scaling agrees with our numerical calculations and Fig. 1.

Because of the similarity between matrix elements (22) and (23) of operators $V^{\rm CP,EDM}$ and $V^{\rm CP,NC}$, there is no need in calculating independently the NC contribution to $\beta^{\rm CP}$. It is sufficient to substitute matrix elements (22) in all equations with matrix elements (23). Comparing these expressions we find that to get the contribution to $\beta^{\rm CP}$ induced by the CP-odd weak neutral currents we need to make following substitution:

$$\frac{d_e}{er_0} \Longleftrightarrow 0.64\times 10^{-13}\frac{R^{\rm NC}}{R^{\rm EDM}}k_1^{\rm nuc}, \qquad (26)$$

where r_0 is the Bohr radius and $R^{\rm EDM}$ and $R^{\rm NC}$ are given by (24) and (25). The accuracy of Eq. (26) is typically 15 – 20%, which is sufficient for our purposes. It was used to calculate the last column of Table I.

IV. LIMITS ON ELECTRON EDM FROM MEASUREMENT OF CP-ODD POLARIZABILITY

Here we envision the following experimental setup (see Fig. 2) to measure the CP-violating polarizability: A strong electric field $\mathcal{E}_0$ is applied to a sample of diamagnetic atoms of number density n. A macroscopic magnetization arises due to the CP-violating polarizability. This magnetization generates a very weak magnetic field B. One could measure this induced magnetic field and set the limits on the electron EDM or other CP-violating mechanisms. In particular, for a spherical cell the maximum value of the generated magnetic field at the surface of the sphere can be related to the CP-violating polarizability as

$$B_{\rm max} = \frac{8\pi}{3} n\,\beta^{\rm CP}\mathcal{E}_0\,. \qquad (27)$$

Clearly, one should increase the number density to enhance the signal, and it is beneficial to work with a dense liquid or solid sample.

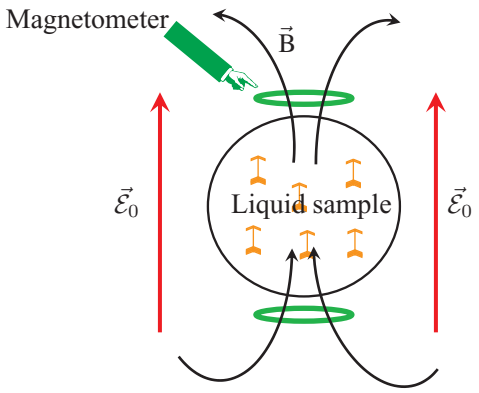

FIG. 2: (Color online) A scheme for measuring CP-violating polarizability.

Among the rare-gas atoms, considered here, xenon has the most suitable properties for such an experiment: Xe is the heaviest non-radioactive atom, it has a large number density ($n \sim 10^{22}\,1/{\rm cm}^3$), and liquid Xe has a high electric field breakdown strength ($\mathcal{E}_0 \sim 4\times 10^5$V/cm). Our calculations in Section III were carried out for isolated atoms. However, in a liquid, there are certain environmental effects (such as confinement of electronic density) that affect the CP-violating signal. To estimate the confinement effects in the liquid, we employ the liquid-cell model. The calculations are similar to those presented in Ref. [16]. In brief, we solve the DHF equations for a Xe atom in a spherical cavity of radius $R_{\rm cav} = \left(\frac{3}{4\pi}\frac{1}{n}\right)^{1/3}$, with certain boundary conditions imposed at the cavity surface. For a density of LXe of 500 amagat [17], $R_{\rm cav} \simeq 4.9$ bohr. For a solid state, $R_{\rm cav} \simeq 4.2$ bohr and we use the latter in the calculations (see discussion in Ref. [16]). Technically, we applied

the variational Galerkin method on a set of 100 B-spline functions [15]. We find numerically that compared to an isolated atom, the CP-violating polarizability of a Xe atom in LXe is reduced by about 65%,

$$\beta^{\rm CP}({\rm LXe}) \approx 1.5 \times 10^{-2} d_e \,. \tag{28}$$

From Eq. (27) it is clear that the more sensitive the measurement of the B-field, the tighter the constraints on $\beta^{\rm CP}$ (and d_e) are. Presently, the most sensitive measurement of weak magnetic fields has been carried out by Princeton group [18]. Using atomic magnetometry, this group has reached the sensitivity level of $5.4 \times 10^{-12}\,{\rm G}/\sqrt{\rm Hz}$. The projected theoretical limit [18] of this method is $10^{-13}\,{\rm G}/\sqrt{\rm Hz}$. Notice that this estimate has been carried out for a sample of volume 0.3 $\rm cm^3$. According to Romalis [19], the sensitivity increases with volume V as $V^{1/3}$, so a 100 $\rm cm^3$ cell would have an even better sensitivity of about $10^{-14}\,{\rm G/Hz}^{1/2}$. More optimistic estimate, based on nonlinear Faraday effect in atomic vapors [20], is given in Ref.[21]; here the projected sensitivity is $3 \times 10^{-15}\,{\rm G}/\sqrt{\rm Hz}$.

Assuming 10 days of averaging, the most optimistic published estimate of the sensitivity to magnetic field [21] leads to the weakest measurable field of $B \simeq 3 \times 10^{-18}\,{\rm G}$. Combining this estimate with the breakdown strength of the E-field for LXe, $\mathcal{E}_0 \sim 4 \times 10^5\,{\rm V/cm}$, and our computed value of CP-odd polarizability, Eq. (28), we arrive at the constraint on the electron EDM,

$$d_e({\rm LXe}) < 6 \times 10^{-26}\, e \cdot {\rm cm}. \tag{29}$$

This projected limit is more than an order of magnitude worse than the present limit on the electron EDM from the Tl experiment [7], $d_e\,({\rm Tl}) < 1.6 \times 10^{-27}\, e \cdot {\rm cm}$. It is worth emphasizing that the above limit has been obtained using B-field sensitivity estimate from Ref. [21]; with the present sensitivity record [18], the constraints of electron EDM are several orders of magnitude weaker. In other words, we find that a substantial improvement in the experimental sensitivity to weak magnetic fields is required before the CP-violating polarizability of LXe can be used for EDM searches.

V. CONCLUSION

To summarize, we have computed novel CP-violating atomic polarizabilities [3], $\beta^{\rm CP}$, for rare-gas atoms. We have derived third-order expressions for $\beta^{\rm CP}$ and employed the Dirac-Hartree-Fock method to evaluate the resulting expressions. We have elucidated the doubly relativistic origin of the polarizability and demonstrated strong Z^5 dependence on the nuclear charge. Finally, we evaluated a feasibility of setting a limit on the electron EDM by measuring CP-violating magnetization of liquid Xe. We found that such an experiment could provide competitive bounds on electron EDM only if the present level of experimental sensitivity to ultra-weak magnetic fields [18] is improved by several orders of magnitude.

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